IRIA

CENTRE DE ROCQUENCOURT

Institut National
de Recherche
en Informatique
et en Automatique

Domaine de Voluceau
Rocquencourt
B.P.105
78153 Le Chesnay Cedex
France
Tél. 954 90 20

Rapports de Recherche

N° 176

SINGULAR PERTURBATIONS AND FINITE ELEMENTS FOR THE NUMERICAL SIMULATION OF SOME PROBLEMS IN V.L.S.I.

Enrique FERNANDEZ CARA

Décembre 1982

SINGULAR PERTURBATIONS AND FINITE ELEMENTS FOR THE NUMERICAL SIMULATION OF SOME PROBLEMS IN V.L.S.I.

Enrique FERNANDEZ CARA(*)

RESUME : Ce papier est consacré à la résolution numérique de quelques problèmes de diffusion non linéaires intervenant en physique des semi-conducteurs, liés à des phénomènes de ségrégation d'impuretés. Nous décrivons d'abord les problèmes physiques non stationnaires, qui conduisent à des équations paraboliques non linéaires couplées par des conditions de transmission et dépendant d'un paramètre $\varepsilon > 0$. Ensuite nous introduisons quelques schémas de discrétisation dans le temps et nous analysons le comportement des solutions correspondantes. On établit ainsi la convergence de ce procédé d'approximation. Pour la résolution numérique, nous formulons un problème approché (éléments finis P_1 Lagrange) qui peut se résoudre par des méthodes de perturbations singulières. Finalement, nous présentons quelques expériences numériques concernant un exemple particulier intervenant dans la technologie.

ABSTRACT : This paper deals with the numerical solution of some nonlinear diffusion problems arising in semi-conductor process modelling and related to impurity segregation phenomena. First, we describe the physical non-stationary problems, which lead to nonlinear parabolic equations coupled by transmission conditions and depending on a parameter $\varepsilon > 0$. Next some time discretization schemes are introduced and we analyze the behaviour of the corresponding solutions. The convergence of this procedure is thus established. For the numerical solution, we use a standard (P_1 Lagrange) finite element approximation, combined with singular perturbation methods. Some numerical experiments are presented for one important example arising in the technology.

(*) I.N.R.I.A. - Domaine de Voluceau - Rocquencourt - B.P. 105 - 78153 LE CHESNAY Cedex.

Contents

INTRODUCTION : THREE PARTICULAR PROBLEMS ARISING IN THE TECHNOLOGY OF V.L.S.I. PROCESSES

This paper is concerned with the numerical simulation of impurity diffusion and segregation phenomena in semiconductor process modelling. For simplicity, we will only consider the two-dimensional nonlinear diffusion of one impurity in silicon, provided an "old" impurity distribution has already been implanted. To extend the results to three-dimensional situations, only some technical arguments are required. On the other hand, an extension of the methods to coupled diffusion problems is also possible (see [2]).

The geometry of an idealized structure is displayed in Fig. 1, where Ω_1 is filled by silicon and Ω_2 represents the oxide mask. Denoting by u (resp. v) the concentration of the "new" impurity in the domain Ω_1 (resp. Ω_2) it is a well-known fact that u is governed by the continuity equation

$$\frac{\partial u}{\partial t} - \nabla\cdot(D_1(u)\nabla u) = 0 \text{ in } \Omega_1 \times (0,T) \tag{1.1}$$

(where the diffusion coefficient D_1 is explicitely given in Appendix A for impurities as arsenic and Boron), while v satisfies the linear equation

$$\frac{\partial v}{\partial t} - \varepsilon D_2 \Delta v = 0 \quad \text{in} \quad \Omega_2 \times (0,T) \ , \tag{1.2}$$

with ε and D_2 being positive constants. In practice ε is small with respect to the other orders of magnitude arising in the problem. For geometrical data as in Fig. 1, the equations (1.1)-(1.2) can be completed with different sets of boundary, transmission and initial conditions. It will be sufficient to our purposes to consider the following three particular problems :

Problem (P_ε) : Find a couple $(u_\varepsilon, v_\varepsilon)$ satisfying the continuity equations (1.1)-(1.2) together with the boundary conditions

$$(BC)_1 \qquad \begin{cases} u = c_o \ \underline{\text{on}} \ \Gamma_1^h \ , \ u = o \ \underline{\text{on}} \ \Gamma_1^f \ , \\ v = c_o \ \underline{\text{on}} \ \Gamma_2^h \ , \end{cases}$$

$$(BC)_2 \qquad \begin{cases} \dfrac{\partial u}{\partial n_1} = o \ \underline{\text{on}} \ \Gamma_1^\ell \ , \\ \dfrac{\partial v}{\partial n_2} = o \ \underline{\text{on}} \ \Gamma_2^\ell \ , \end{cases}$$

the interface (or transmission) conditions

$$(SC) \qquad u = mv \quad , \quad D_1(u)\frac{\partial u}{\partial n_1} = -\varepsilon D_2 \frac{\partial v}{\partial n_2} \quad \underline{on} \quad S \ ,$$

and the initial-value conditions

$$(IVC)_1 \qquad u_{|t=o} = o \quad \underline{in} \quad \Omega_1 \ , \quad v_{|t=o} = o \quad \underline{in} \quad \Omega_2 \ . \qquad \square$$

Problem (Q_ε) : Find a couple $(u_\varepsilon, v_\varepsilon)$ satisfying (1.1)-(1.2) together with the boundary conditions $(BC)_2$ and

$$(BC)_3 \qquad \begin{cases} \dfrac{\partial u}{\partial n_1} = o \quad \underline{on} \quad \Gamma_1^h \ , \\ u = o \quad \underline{on} \quad \Gamma_1^f \ , \end{cases}$$

the transmission conditions (SC) and the initial-value conditions

$$(IVC)_2 \qquad u_{|t=o} = o \quad \underline{in} \quad \Omega_1 \ , \quad v_{|t=o} = C_o \quad \underline{in} \quad \Omega_2 \ . \qquad \square$$

Problem (R_ε) : Find a couple $(u_\varepsilon, v_\varepsilon)$ satisfying (1.1)-(1.2) together with the boundary conditions $(BC)_2$-$(BC)_3$, conditions (SC) on S and the initial-value conditions

$$(IVC)_3 \qquad u_{|t=o} = u_o \quad \underline{in} \quad \Omega_1 \ , \quad v_{|t=o} = v_o \quad \underline{in} \quad \Omega_2 \ . \qquad \square$$

In $(BC)_1$, (SC), $(IVC)_1$ and $(IVC)_2$, C_o and m are positive constants and the functions u_o and v_o in $(IVC)_3$ are assumed to verify :

$$(1.3) \qquad \begin{cases} u_o \in L^2(\Omega_1) \ , \quad v_o \in L^2(\Omega_1) \ , \\ u_o, v_o \geq 0 \ , \quad u_o \not\equiv o \ , \quad v_o \not\equiv o \ . \end{cases}$$

These three problems model different important V.L.S.I. processes. For problem (P_ε), impurities are introducted in Ω_1 and Ω_2 directly from outside

They enter the silicon (resp. the oxide) through the window Γ_1^h (resp. Γ_2^h), where the concentration level is held at a constant value. The transmission conditions (SC) are the consequence of assumptions of continuity for the chemical potential(*) and the impurity flux and, for this problem, clearly lead to a discontinuity in x_c (see Fig. 1).

In problem (Q_ε), impurities are initially localized inside the mask (again at constant concentration C_o), which plays the role of a finite reservoir. They enter the silicon through the interface S. This happens also in (R_ε), but now initial non zero impurity are imposed in both media. In all cases, the Neumann's conditions $(BC)_2$ account for the symmetry of the geometrical data, while the Dirichlet condition on Γ_1^f just says that for $t \leq T$ impurities do not fill Ω_1.

As in [6, 7], standard methods can be used to show that problems (Q_ε) and (R_ε) possess exactly one solution $(u_\varepsilon, v_\varepsilon)$, also satisfying

$$
(1.4) \qquad \begin{cases} u_\varepsilon \in L^2(0,T\ ;\ H^1(\Omega_1)) \cap L^\infty(0,T\ ;\ L^2(\Omega_1)) \ , \\ v_\varepsilon \in L^2(0,T\ ;\ H^1(\Omega_2)) \cap L^\infty(0,T\ ;\ L^2(\Omega_2)) \ , \\ \dfrac{\partial u_\varepsilon}{\partial t} \in L^2(0,T\ ;\ V_1') \ , \ \dfrac{\partial v_\varepsilon}{\partial t} \in L^2(0,T\ ;\ V_2') \ , \end{cases}
$$

where

$$
V_i = \{\phi \,|\, \phi \in H^1(\Omega_i)\ ;\ \phi = 0 \ \underline{\text{on}}\ \Gamma_i^b\}
$$

and

$$
\Gamma_1^b \equiv \Gamma_1^f \ , \quad \Gamma_2^b \equiv \Gamma_2^f = \emptyset \ .
$$

(*) This is actually the physical assumption leading to the segregation phenomenon. The constant m is taken equal to 10. for acceptors as boron and equal to .10 for donnors as arsenic (see e.g. [2,5,12]).

For problem (P_ε) the situation is more complicate. Indeed the boundary conditions $(BC)_1$ and conditions (SC) together lead to a singularity at x_c. However, a desingularization procedure can be used to show that problem (P_ε) possesses exactly one solution again satisfying (1.4) with

$$\Gamma_1^b \equiv \Gamma_1^f \cup \Gamma_1^h \quad , \quad \Gamma_2^b \equiv \Gamma_2^h$$

(see [7]).

In all the sequel, for a couple $(u,v) \in H^1(\Omega_1) \times H^1(\Omega_2)$ we will denote by $U = \{u,v\}$ the function (a.e. defined in Ω) given by

$$U = \begin{cases} u \ \underline{\text{in}} \ \Omega_1, \\ v \ \underline{\text{in}} \ \Omega_2 . \end{cases}$$

2. - THE SEMI-DISCRETIZED PROBLEM (I) : EXISTENCE AND UNIQUENESS RESULTS

To solve problems (P_ε), (Q_ε) and (R_ε), it is useful to introduce some time discretization schemes. Roughly speaking, the procedure consists in substituting the time derivative operator $\frac{\partial}{\partial t}$ by a finite difference operator leading to a sequence of nonlinear elliptic problems. This Section deals with the existence and uniqueness of solution for these problems.

Let us consider (say) equation (1.1). Some schemes with step $\tau > 0$ in the variable t read as follows :

i) Implicit scheme :

$$\frac{u^{n+1} - u^n}{\tau} - \nabla\cdot(D_1(u^{n+1})\nabla u^{n+1}) = 0 \ \underline{\text{in}} \ \Omega_1 . \tag{2.1}$$

ii) Gear's scheme :

$$\frac{3}{2}\left(\frac{u^{n+1} - u^n}{\tau}\right) - \frac{1}{2}\left(\frac{u^n - u^{n-1}}{\tau}\right) - \nabla\cdot(D_1(u^{n+1})\nabla u^{n+1}) = 0 \ \underline{\text{in}} \ \Omega_1 . \tag{2.2}$$

iii) Crank-Nicholson's scheme :

$$(2.3) \qquad \frac{u^{n+1} - u^n}{\tau} - \nabla\cdot(D_1(u^{n+1/2})\nabla u^{n+1/2}) = 0 \quad \underline{\text{in}} \quad \Omega_1 .$$

Here, for $s \in \mathbb{R}_+$, u^s is an approximation of $u(s\tau)$, with (u,v) being the solution of the problem. In (2.1) and (2.2) the unknown is u^{n+1}, while u^n (and also u^{n-1} in (2.2)) is given : it was computed at the previous time step. In (2.3), $u^{n+1/2}$ is unknown and u^n, u^{n+1} are given. In practice, it is more convenient to use the previous schemes with variable time step τ_n. In particular, for (2.2) the following approximation appears for the term $\frac{\partial u}{\partial t}$ in (1.1) at $t = \sum_{i=1}^{n+1} \tau_i$:

$$(2.4) \qquad \frac{2\tau_n + \tau_{n+1}}{\tau_n(\tau_n + \tau_{n+1})} u^{n+1} - \frac{\tau_n + \tau_{n+1}}{\tau_n \tau_{n+1}} u^n + \frac{\tau_n}{(\tau_{n+1} + \tau_n)\tau_{n+1}} u^{n-1} .$$

In the sequel, and except in Section 6, we will concentrate our attention on implicit schemes. Most of arguments which follow are also valid for other schemes, and a numerical comparison of their performance is given in [2].

Thus, given a positive parameter $\tau > 0$, we are led to some nonlinear elliptic problems which read :

Problem (P_ε^n) : Find a couple $(u_\varepsilon^{n+1}, v_\varepsilon^{n+1})$ satisfying :

$$(2.4) \qquad -\tau\nabla\cdot(D_1(u_\varepsilon^{n+1})\nabla u_\varepsilon^{n+1}) + u_\varepsilon^{n+1} = u_\varepsilon^n \quad \underline{\text{in}} \quad \Omega_1 ,$$

$$(2.5) \qquad -\tau\varepsilon D_2 \Delta v_\varepsilon^{n+1} + v_\varepsilon^{n+1} = v_\varepsilon^n \quad \underline{\text{in}} \quad \Omega_2 ,$$

together with the boundary conditions $(BC)_1$, $(BC)_2$, and conditions (SC) on S.

□

Problem (Q_ε^n) : Find a couple $(u_\varepsilon^{n+1}, v_\varepsilon^{n+1})$ satisfying (2.4)-(2.5), together with the boundary conditions $(BC)_2$, $(BC)_3$ and conditions (SC) on S.

□

We have the following result :

THEOREM 1. - Let $\varepsilon > 0$, $\tau > 0$ and $U_\varepsilon^n = \{u_\varepsilon^n, v_\varepsilon^n\}$ be given, with

$$(2.6)\qquad \begin{cases} u_\varepsilon^n \in H^1(\Omega_1) \quad , \quad v_\varepsilon^n \in H^1(\Omega_2) \ , \\ 0 \le u_\varepsilon^n \le \tilde{C}_o \quad \underline{\text{a.e. in}} \quad \Omega_1 \quad , \quad \tilde{C}_o \equiv C_o \cdot \max(1,m), \\ 0 \le m v_\varepsilon^n \le \tilde{C}_o \quad \underline{\text{a.e. in}} \quad \Omega_2 \ . \end{cases}$$

Then problem (Q_ε^n) possesses exactly one solution $(u_\varepsilon^{n+1}, v_\varepsilon^{n+1})$, furthermore satisfying :

$$(2.7)\qquad \tilde{U}_\varepsilon^{n+1} \equiv \{u_\varepsilon^{n+1}, m v_\varepsilon^{n+1}\} \in H^1(\Omega) \cap C^{o,\gamma}(\bar{\Omega})$$

for a certain $\gamma \in (0,1)$ and

$$(2.8)\qquad 0 \le U_\varepsilon^{n+1} \le \tilde{C}_o \quad \underline{\text{in}} \quad \Omega.$$

The proof is analogous to the proof of Theorem 1 in [7], and for simplicity only a sketch of it is given below. Notice that for problems (P_ε^n) a singularity occurs again at x_c, which makes the derivation of a similar result much harder (see [7] for a related result).

Sketch of the proof :

1st Part. Existence of solutions (I) : A fixed-point approach.

Let $\mathcal{B}$ be the closed convex set in $C^o(\bar{\Omega}_1)$:

$$\mathcal{B} = \{W \mid W \in C^o(\bar{\Omega}_1) \ ; \ 0 \le W \le \tilde{C}_o \quad \text{in} \quad \bar{\Omega}_1\} \ .$$

For given $a \in \mathcal{B}$, we will say that the couple $(u,v) \in H^1(\Omega_1) \times H^1(\Omega_2)$ solves problem $(Q_\varepsilon - W)$ if it satisfies :

$$(2.9)\qquad -\tau \nabla \cdot (D_1(W) \nabla u) + u = u_\varepsilon^n \quad \underline{\text{in}} \quad \Omega_1 \ ,$$

$$(2.10)\qquad -\tau \varepsilon D_2 \Delta v + v = v_\varepsilon^n \quad \underline{\text{in}} \quad \Omega_2 \ ,$$

together with $(BC)_2$, $(BC)_3$ and (SC). Obviously, for every $W \in \mathcal{B}$, problem $(Q_\varepsilon - W)$ possesses exactly one solution (u,v), furthermore verifying

$$\tilde{U} \equiv \{u, mv\} \in H^1(\Omega)$$

and, by virtue of the maximum principle,

$$0 \leq \tilde{U} \leq \tilde{C}_o \quad \underline{\text{a.e. in}} \quad \Omega. \tag{2.11}$$

We can adapt some results from G. Stampacchia [15] to show that $\tilde{U}$ also satisfies the regularity property :

$$\tilde{U} \in C^{o,\gamma}(\bar{\Omega})$$

for a $\gamma \in (0,1)$. Furthermore, the mapping $W \to u$ is completely continuous from $\mathcal{B}$ into itself. Thus Schauder's Fixed-Point Theorem applies, and a solution $(u_\varepsilon^{n+1}, v_\varepsilon^{n+1})$ of (Q_ε^n) exists. □

Remark 2.1. : The previous arguments readily suggests a first iterative method for solving (P_ε^n) :

Algorithm (A_1) :

a) For $m = 0$, choose $u^{n,o} \in \mathcal{B}$.

b) Then, for given $m \geq 0$ and $u_\varepsilon^{n,m} \in \mathcal{B}$, compute the solution (u,v) of problem $(Q_\varepsilon - u_\varepsilon^{n,m})$ and take $u_\varepsilon^{n,m+1} = u$. □

2^{nd} Part : Existence of solutions (II) : A variational equality.

Let $\tilde{D}_1$ be the truncated diffusion coefficient given by

$$\tilde{D}_1(S) = \begin{cases} D_1(\tilde{C}_o) & \text{if} \quad s \geq \tilde{C}_o \ , \\ D_1(s) & \text{if} \quad 0 < s < \tilde{C}_o \ , \\ D_1(o) & \text{if} \quad s \leq 0 \ , \end{cases} \tag{2.12}$$

and set

$$W = \{\Phi \mid \Phi = \{\phi,\Psi\} \in H^1(\Omega) \ ; \ \phi = 0 \ \underline{\text{on}} \ \Gamma_1^f\} \ , \tag{2.13}$$

$$\tilde{W} = \{\Phi \mid \Phi = \{\phi,\Psi\} \ ; \ \{\phi,m\Psi\} \in W\} \ .$$

We consider the variational equality

$$\left\{ \begin{array}{l} \displaystyle\int_{\Omega_1} u\phi + \tau\int_{\Omega_1} D_1(u)\nabla u\cdot\nabla\phi \ + \int_{\Omega_2} v\Psi \ + \tau\varepsilon D_2\int_{\Omega_2} \nabla v\cdot\nabla\psi = \int_{\Omega_1} u_\varepsilon^n\phi + \int_{\Omega_2} v_\varepsilon^n\Psi \\ \\ \forall\Phi = \{\phi,\Psi\} \in W \ , \quad U = \{u,v\} \in \tilde{W}. \end{array} \right. \tag{2.15}$$

The compactness method of J.L. Lions [13] can be adapted here to show that (2.15) possesses at least one solution $U_\varepsilon^{n+1} = \{u_\varepsilon^{n+1}, v_\varepsilon^{n+1}\}$. Remark that (2.8) must hold, according to the maximum principle for second order elliptic problems (see [15]). Hence U_ε^{n+1} is a solution of (Q_ε^n). □

Remark 2.2. - A direct (global) finite element approximation of (Q_ε^n) can be readily obtained from the equality (2.15) (see Section 5). □

3rd Part : Uniqueness of solution.

Let (u,v) and $(\tilde{u},\tilde{v})$ be two solutions of (Q_ε^n). Then

$$0 = \int_{\Omega_1} |(u-\tilde{u}) - \tau\nabla\cdot(D_1(u)\nabla u - D_1(\tilde{u})\nabla\tilde{u})| + \int_{\Omega_2} |(v-\tilde{v}) - \varepsilon D_2\Delta(v-\tilde{v})| \tag{2.16}$$

Adapting a method due to M.G. Crandall [4], it is not hard to see that left-hand side in (2.16) is bounded from below by

$$\int_{\Omega_1} |u-\tilde{u}| + \int_{\Omega_2} |v-\tilde{v}| \ .$$

This yields uniqueness for the solution of (Q_ε^n). □

3. - THE SEMI-DISCRETIZED PROBLEM (II) : A CONVERGENCE RESULT

We turn now to the proof of some convergence properties of the solutions of the semi-discretized problems as $\tau \downarrow 0$. For each fixed $\tau > 0$ ($T = N\tau$, with $N \geq 1$ being an integer), we associate to the solution $U^1, U^2, \ldots, U^{N(*)}$ the approximate functions $\tilde{U}_\tau \equiv \{u_\tau, mv_\tau\}$ and $U_\tau^* \equiv \{u_\tau^*, mv_\tau^*\}$, given by

$$\tilde{U}_\tau(t) = \tilde{U}^n \equiv \{u^n, mv^n\} \quad \text{for } t \in [(n-1)\tau, n\tau], \; n = 1, 2, \ldots, N, \tag{3.1}$$

$$\begin{cases} U_\tau^*(t) \text{ is continuous, linear on each interval } [(n-1)\tau, n\tau], \text{ and} \\ U_\tau^*(n\tau) = \tilde{U}^n \quad \text{for} \quad n = 0, \; , \ldots, N. \end{cases} \tag{3.2}$$

Our main result in this Section is the following :

THEOREM 2 : Let the functions $\tilde{U}_\tau$ and U_τ^* be defined as in (3.1), (3.2) for every $\tau > 0$, with (u^n, v^n) being the solution of (Q^n) for $n = 1, 2, \ldots, N$. Then one has :

$$\tilde{U}_\tau \to \tilde{U} \text{ and } U_\tau^* \to \tilde{U} \quad \text{weakly in} \quad L^2(0,T ; H^1(\Omega)) \quad \text{and} \quad L^\infty(\Omega \times (0,T))*$$

$$U_\tau^* \to \tilde{U} \quad \text{strongly in} \quad L^2(\Omega \times (0,T)) \quad \text{and a.e.},$$

$$\frac{\partial U_\tau^*}{\partial t} \to \frac{\partial U}{\partial t} \quad \text{weakly in} \quad L^2(0,T ; W') \; ,$$

where $\tilde{U} \equiv \{u, mv\}$, with (u,v) being the (unique) solution of (Q).

For the proof, we prepare the following Lemma, which will further lead to some "a priori" estimates.

LEMMA 3.1 : There exists three constants C_2, C_3 and C_4, only depending on C_o , $D_1(\cdot)$, ε, D_2, T, m and Ω such that the following inequalities hold :

(*) In this Section we omit the subscript ε. Recall that $U^n = \{u^n, v^n\}$, with (u^n, v^n) being the solution of (Q^n).

$$\|\{u^n, mv^n\}\|_{L^\infty} \le \tilde{C}_o \quad , \tag{3.3}$$

$$\tau \sum_{n=1}^{N} \|\{u^n, mv^n\}\|_{H^1} \le C_2 \quad , \tag{3.4}$$

$$\sum_{n=1}^{N} \|U^n - U^{n-1}\|_{L^2}^2 \le C_3 \quad , \tag{3.5}$$

$$\tau \sum_{n=1}^{N} \left\|\frac{U^n - U^{n-1}}{\tau}\right\|^2 \le C_4 \ . \tag{3.6}$$

Proof : The first inequality is directly given by (2.8). Let us prove (3.4) and (3.5). Notice that

$$\int_{\Omega_1} (u^{n+1} - u^n)u^{n+1} + m \int_{\Omega_1} (v^{n+1} - v^n)v^{n+1}$$
$$+ \tau \int_{\Omega_1} D_1(u^{n+1}) |\nabla u^{n+1}|^2 + \tau\varepsilon D_2 \int_{\Omega_2} |\nabla v^{n+1}|^2 = 0 \ .$$

Using the identity

$$2(a-b)a = a^2 - b^2 + |a-b|^2 \qquad \forall a,b \in \mathbb{R} \ ,$$

one obtains :

$$\frac{1}{2}\|U^{n+1}\|_{L^2}^2 - \frac{1}{2}\|U^n\|_{L^2}^2 + \frac{1}{2}\|U^{n+1} - U^n\|_{L^2}^2 + \tau\|U^{n+1}\|_{H^1}^2 \le \tau C_4 \ , \tag{3.7}$$

where $C_4 > 0$ depends on $D_1(\cdot)$, ε, D_2, m and Ω, but is independent from τ. Summing the equalities (3.7) for n = 1, 2, ..., N-1, we find :

$$\frac{1}{2}\|\tilde{U}^N\|_{L^2}^2 - \frac{1}{2}\|\tilde{U}^1\|_{L^2}^2 + \frac{1}{2}\sum_{n=1}^{N-1} \|\tilde{U}^{n+1} - \tilde{U}^n\|_{L^2}^2 + \tau \sum_{n=2}^{N} \|\tilde{U}^n\|_{H^1}^2 \le C_4' \tag{3.8}$$

whith $C_4' = (N-1)\tau C_4 < TC_4$. On the other hand, by definition, (u^1, v^1) satisfies :

$$\int_{\Omega_1} u^1\Psi + \int_{\Omega_2} v^1\phi + \tau\int_{\Omega_1} D_1(u^1)\nabla u^1 \cdot \nabla\phi + \tau\varepsilon D_2 \int_{\Omega_2} \nabla v^1 \cdot \nabla\Psi = 0$$

for all $\Phi = \{\phi,\Psi\} \in W$. This yields

$$\|\tilde{U}^1\|^2_{L^2} + \tau\|\tilde{U}^1\|^2_{H^1} \leq C_5 \quad , \tag{3.9}$$

where again C_5 only depends on $D_1(\cdot)$, ε, D_2, m and Ω. From (3.8)-(3.9) we easily obtain (3.4) and (3.5).

In order to prove (3.6) we remark that

$$\|U^n - U^{n-1}\|_{L^2} = \sup_{\substack{\Phi=\{\phi,\Psi\}\in W \\ \|\Phi\|_{H^1}\leq 1}} \{\int_{\Omega_1} (u^n - u^{n-1})\phi + \int_{\Omega_2} (v^n - v^{n-1})\Psi\}$$

$$= \tau \sup_{\substack{\Phi\in W \\ \|\Phi\|_{H^1}\leq 1}} \{\int_{\Omega_1} D_1(u^n)\nabla u^n\cdot\nabla\phi + \varepsilon D_2 \int_{\Omega_2} \nabla v^n\cdot\nabla\Psi\}$$

$$\leq \tau\, C_6\|\tilde{U}^n\|_{H^1} \quad .$$

This inequality, together with (3.4), imply (3.6). □

Proof of Theorem 2

1st Step : Some "a priori" estimates

From (3.3)-(3.6), one sees that $\tilde{U}_\tau$ and U^*_τ satisfy the following properties as $\tau \to 0$:

(3.11a) $\tilde{U}_\tau, U^*_\tau$ are uniformly bounded in $L^2(0,T\,;\,H^1(\Omega)) \cap L^\infty(\Omega\times(0,T))$,

(3.11b) $\dfrac{\partial U^*_\tau}{\partial t}$ is uniformly bounded in $L^2(0,T\,;\,W')$

We also notice that the following identity holds for $n = 1,2,\ldots,N$:

$$\int_{(n-1)\tau}^{n\tau} \int_\Omega |U^*_\tau(t) - \tilde{U}_\tau(t)|^2\, dt = \frac{\tau}{3}\int_\Omega |\tilde{U}^n - \tilde{U}^{n-1}|^2 \quad .$$

Hence,

$$\|\tilde{U}_\tau - U_\tau^*\|^2_{L^2(\Omega \times (0,T))} = \frac{\tau}{3} \sum_{n=1}^{N} \|\tilde{U}^n - \tilde{U}^{n-1}\|^2_{L^2} ,$$

and from (3.5) we deduce that a subsequence $\tilde{U}_\sigma$ exists for which

(3.12a) $\quad U_\sigma^* - \tilde{U}_\sigma \to 0$ <u>strongly in</u> $L^2(\Omega \times (0,T))$

as $\sigma \to 0$. □

<u>2nd Step : Passage to the limit</u>

From (3.11a)-(3.11b) and (3.12a), there exists a subsequence (again indexed by σ) such that :

(3.12b) $\quad \tilde{U}_\sigma \to \tilde{U}$, $U_\sigma^* \to \tilde{U}$ <u>weakly in</u> $L^2(0,T ; H^1(\Omega))$ and $L^\infty(\Omega \times (0,T))*$

(3.12c) $\quad \frac{\partial U_\sigma^*}{\partial t} \to \frac{\partial U}{\partial t}$ <u>weakly in</u> $L^2(0,T ; W')$.

Let us put $\tilde{U} = \{u, mv\}$. We only have to prove that (u,v) solves problem (Q). But from (3.12b)-(3.12c) we obtain

(3.12d) $\quad U_\sigma^* \to \tilde{U}$ <u>strongly in</u> $L^2(\Omega \times (0,T))$,

and now (3.12a) yields :

(3.12e) $\quad \tilde{U}_\sigma \to \tilde{U}$ <u>strongly in</u> $L^2(\Omega \times (0,T))$.

On the other hand, we can rewrite problems (Q_n) globally as

(3.13) $$\{\frac{\partial u_\tau^*}{\partial t} , \frac{\partial v_\tau^*}{\partial t}\} - \{\nabla\cdot(D_1(u_\tau)\nabla u_\tau) , \varepsilon D_2 \Delta v_\tau\} = 0 .$$

By virtue of (3.12), one can pass to the limit in (3.13) which leads to :

$$\{\frac{\partial u}{\partial t} , \frac{\partial v}{\partial t}\} - \{\nabla\cdot(D(u)\nabla u) , \varepsilon D_2 \Delta v\} = 0 .$$

Due to (3.12b)-(3.12c) and the fact that $U_\tau^*(0) = U^0 \equiv 0$, we finally obtain :

$$u_{|t=0} = 0 \text{ in } \Omega_1 \ , \ v_{|t=0} = 0 \text{ in } \Omega_2 \ .$$

Thus, (u,v) is the (unique) solution of (Q). □

Remark 3.1 : For problem (P) a similar result can be derived. Furthermore, these arguments also provide a proof of the existence of solutions of the nonstationary problem (see [ ]). □

4. - A SINGULAR PERTURBATION APPROACH FOR THE SOLUTION OF THE SEMI-DISCRETIZED PROBLEMS

The main result in Section 3 (Theorem 2) has an important consequence : to compute the solution of problem (Q_ε) it is appropriate to solve (Q_ε^n) for small $\tau = T/N$ and $n = 0, 1, \ldots, N$. Thus the task consists in solving a finite set of nonlinear elliptic problems. A first (global) finite element discretization is introduced in Section 5 ; in some particular cases it may be inappropriate, due to the different orders of magnitude of the diffusion coefficients corresponding to subdomains Ω_1 and Ω_2, and to the coupling transmission conditions on S. An alternative is provided by the singular perturbation approach described in this Section. This method, combined with a finite (P_1 Lagrange) element discretization, has proved quite efficient from the numerical wiewpoint. (See Section 6). For simplicity, a description of it will be given in the framework of the continuous problem (Q_ε).

Let $(u_\varepsilon, v_\varepsilon)$ be the solution of (Q_ε^n). We introduce the formal series

$$U_\varepsilon \equiv \{u_\varepsilon, v_\varepsilon\} = \frac{U^{-1}}{\varepsilon} + U^0 + \varepsilon U^1 + \varepsilon^2 U^2 + \ldots \ , \tag{4.1}$$

where the (unknown) functions $U^r = \{u^r, v^r\}$ are required to satisfy

$$U^r \in \tilde{W} \qquad \forall r \geq -1 \ . \tag{4.2}$$

Since a singularity occurs exclusively in Ω_2 as $\varepsilon \to 0$ (see e.g. [7]), and by analogy with linear stiff problems (cf. J.L. LIONS [14]), it seems

reasonable to assume

$$u^{-1} = 0.$$

Thus, the identification of the powers of ε in (4.1) yields :

a) $U^{-1} = \{o, v^{-1}\}$, with v^{-1} being the (unique) solution of the linear problem

$$(4.3) \qquad \begin{cases} -\tau\varepsilon D_2 \Delta v^{-1} + v^{-1} = \varepsilon v_\varepsilon^n \ \underline{\text{in}}\ \Omega_2 \ , \\ \dfrac{\partial v^{-1}}{\partial n_2} = 0 \ \underline{\text{on}}\ \Gamma_2 \cup \Gamma_2^\ell \ , \\ v^{-1} = 0 \ \underline{\text{on}}\ S. \end{cases}$$

b) $U^o = \{u^o, v^o\}$, where u^o is the solution of the nonlinear problem

$$(4.4)_1 \qquad \begin{cases} -\tau\nabla\cdot(D_1(u^o)\nabla u^o) + u^o = u_\varepsilon^n \ \underline{\text{in}}\ \Omega_1 \ , \\ \dfrac{\partial u^o}{\partial n_1} = 0 \ \underline{\text{on}}\ \Gamma_1^h \cup \Gamma_1^\ell \ , \quad u^o = 0 \ \underline{\text{on}}\ \Gamma_1^f \ , \\ D_1(u^o)\dfrac{\partial u^o}{\partial n_1} = -D_2 \dfrac{\partial v^{-1}}{\partial n_2} \ \underline{\text{on}}\ S \ , \end{cases}$$

and v^o is the solution of the linear problem

$$(4.4)_2 \qquad \begin{cases} -\tau\varepsilon D_2 \Delta v^o + v^o = 0 \ \underline{\text{in}}\ \Omega_2 \ , \\ \dfrac{\partial v^o}{\partial n_2} = 0 \ \underline{\text{on}}\ \Gamma_2^h \cup \Gamma_2^\ell \ , \\ v^o = \dfrac{1}{m} u^o \ \underline{\text{on}}\ S \ . \end{cases}$$

c) $U^{-1} = \{u^1, v^1\}$, where u^1 is the solution of the linear problem

$$(4.5)_1 \qquad \begin{cases} -\tau\Delta(D_1(u^o)u^1) + u^1 = 0 \ \underline{\text{in}}\ \Omega_1 \ , \\ \dfrac{\partial u^o}{\partial n_1} = 0 \ \underline{\text{on}}\ \Gamma_1^h \cup \Gamma_1^\ell \ , \ u^o = 0 \ \underline{\text{on}}\ \Gamma_1^f \ , \\ \dfrac{\partial}{\partial n_1}(D_1(u^o)u^1) = -D_2 \dfrac{\partial v^o}{\partial n_2} \ \underline{\text{on}}\ S \ , \end{cases}$$

and v^1 is the solution of the linear problem

$$(4.5)_2 \qquad \begin{cases} -\tau\varepsilon D_2 \Delta v^1 + v^1 = 0 \quad \underline{\text{in}} \quad \Omega_2 \ , \\ \dfrac{\partial v^{-1}}{\partial n_2} = 0 \quad \underline{\text{on}} \quad \Gamma_2^h \cup \Gamma_2^\ell \ , \\ v^1 = \dfrac{1}{m} u^1 \quad \underline{\text{on}} \quad S \ . \end{cases}$$

etc...

Let us make a few comments on these intermediate problems. First of all, remark that the assumption $u^{-1} = 0$ provides the following ordering in determining the functions U^r :

$$v^{-1} \to u^o \to v^o \to u^1 \to v^1 \to u^2 \to \ldots$$

Furthermore, the "information" which enables us to compute u^r from v^{r-1} lies on the normal derivative $D_2 \dfrac{\partial v^{r-1}}{\partial n_2}$ on S (the normal impurity flux in the simulation of V.L.S.I. processes ; see Section 1), while v^r depends on the trace of u^r at the interface (the impurity concentration on S) via a Dirichlet condition of the segregation type.

It is also observed that only problem $(4.4)_1$ is nonlinear ; this means that the numerical work represents an amount of linear problems with respect to the semi-discretized <u>idealized</u> problem (for which $\varepsilon = 0$; see e.g. [1,3]).

Let us finally mention that this method is easy to adapt to other related problems including interface conditions as (SC). For instance, in the case of problem (P_ε^n), it suffices to replace all Neumann condtions on Γ_1^h and Γ_2^h by :

$$u^r\big|_{\Gamma_1^h} \ , \ v^r\big|_{\Gamma_2^h} = \begin{cases} C_o \ \underline{\text{if}} \ r = 0 \ , \\ 0 \ \underline{\text{otherwise}} \ . \end{cases}$$

In practice, this approach has been carried out up to the term of zero and first order in ε. Of course it could be pushed further, and the derivation of the occurring equations may be an interesting exercice.

5. - DISCRETIZATION IN THE SPACE VARIABLES : A FINITE ELEMENT APPROXIMATION

In this Section we introduce a (P_1 Lagrange) finit element approximation of problems (P_ε^n) and (Q_ε^n) and describe some iterative methods of solution. We also indicate at the end of this Section how the previous singular perturbation techniques in Section 4 combine with a finite element discretization.

Thus, let $\mathcal{C}_h$ be a triangulation of $\bar{\Omega}$ (see e.g. [ ]) such that $\mathcal{C}_{ih} = \{T/T \in \mathcal{C}_h \; ; \; T \subset \bar{\Omega}_i\}$ is a triangulation of Ω_i for i = 1,2. The following finite dimensional spaces will be required :

$$V_{ih} = \{\phi_h/\phi_h \in C^o(\bar{\Omega}_i) \; ; \; \phi_h|_T \in P_1 \quad \forall T \in \mathcal{C}_{ih}\} \; , \tag{5.1}$$

$$V_{1h}^o = \{\phi_h/\phi_h \in V_{1h} \; ; \; \phi_h = 0 \; \underline{\text{on}} \; \Gamma_1^h \cup \Gamma_1^f\} \; , \tag{5.2}$$

$$V_{2h}^o = \{\phi_h/\phi_h \in V_{2h} \; ; \; \phi_h = 0 \; \underline{\text{on}} \; \Gamma_2^h\} \; , \tag{5.3}$$

$$W_h = \{\Phi_h/\Phi_h = \{\phi_h,\Psi_h\} \in V_{1h} \times V_{2h} \; ; \; \phi_h = \Psi_h \underline{\text{on}} \; S \; ; \; \phi_h = 0 \; \underline{\text{on}} \; \Gamma_1^f\}, \tag{5.4}$$

$$\tilde{W}_h = \{\Phi_h/\Phi_h = \{\phi_h,\Psi_h\} \; ; \; \{\phi_h,m\Psi_h\} \in W_h\} \; , \tag{5.5}$$

$$W_h^o = \{\Phi_h/\Phi_h = \{\phi_h,\Psi_h\} \in V_{1h}^o \times V_{2h}^o \; ; \; \phi_h = \Psi_h \underline{\text{at the nodes}} \text{ of } \mathcal{C}_h \; \underline{\text{which belong to}} \; S \cap \Omega\} \; , \tag{5.6}$$

$$\tilde{W}_h^o = \{\Phi_h/\Phi_h = \{\phi_h,\Psi_h\} \; ; \; \{\phi_h,m\Psi_h\} \in W_h^o\} \; . \tag{5.7}$$

Let u_Γ, v_Γ be two functions satisfying :

$$u_\Gamma \in W_{1h} \; , \quad u_\Gamma = \begin{cases} C_o & \underline{\text{on}} \; \Gamma_1^h \\ 0 & \underline{\text{on}} \; \Gamma_1^f \end{cases} \; ,$$

$$v_\Gamma \in V_{2h} \; , \quad v_\Gamma = C_o \; \underline{\text{on}} \; \Gamma_2^h \; ,$$

$$u_\Gamma = m v_\Gamma \; \underline{\text{at the nodes of}} \; \mathcal{C}_h \; \underline{\text{belonging to}} \; \Omega \cap S.$$

A direct (global) approximation of (P_ε^n) is given by :

$$
(5.8)\qquad \begin{cases} \displaystyle\int_{\Omega_1} u_h\phi_h + \tau\int_{\Omega_1} D_1(u_h)\nabla u_h\cdot\nabla\phi_h + \int_{\Omega_2} v_h\psi_h + \tau\varepsilon D_2\int_{\Omega_2}\nabla v_h\cdot\nabla\psi_h \\ \qquad = \displaystyle\int_{\Omega_1} u_\varepsilon^n\phi_h + \int_{\Omega_2} v_\varepsilon^n\psi_h \quad \forall\{\phi_h,\psi_h\}\in W_h^o \ , \\ \{u_h,v_h\}\in\{u_\Gamma,v_\Gamma\}+\tilde{W}_h^o \ . \end{cases}
$$

Analogously, problem (Q_ε^n) can be approximated by

$$
(5.9)\qquad \begin{cases} \displaystyle\int_{\Omega_1} u_h\phi_h + \tau\int_{\Omega_1} D_1(u_h)\nabla u_h\cdot\nabla\phi_h + \int_{\Omega_2} v_h\psi_h + \tau\varepsilon D_2\int_{\Omega_2}\nabla v_h\cdot\nabla\psi_h \\ \qquad = \displaystyle\int_{\Omega_1} u_\varepsilon^n\phi_h + \int_{\Omega_2} v_\varepsilon^n\psi_h \quad \forall\{\phi_h,\psi_h\}\in W_h \ , \\ \{u_h,v_h\}\in\{u_\Gamma,v_\Gamma\}+W_h \ . \end{cases}
$$

Now we turn to the numerical solution of (5.8) and (5.9). Arguing as in [1, 2, 3], we can introduce the following iterate methods :

Algorithm (A_{1h}) (Linearization) - One solves the linear system

$$
\int_{\Omega_1} u_h\phi_h + \tau\int_{\Omega_1} D_1(u_\varepsilon^n)\nabla u_h\cdot\phi_h + \int_{\Omega_2} v_h\psi_h + \varepsilon\tau D_2\int_{\Omega_2}\nabla v_h\cdot\nabla\psi_h
$$
$$
= \int_{\Omega_1} u_\varepsilon^n\phi_h + \int_{\Omega_2} v_\varepsilon^n\psi_h \qquad \forall\{\phi_h,\psi_h\} \ . \qquad \square
$$

Algorithm (A_{2h}) (Fixed-Point method ; see [8]) - We start with $\{u_h^{n+1,0}, v_h^{n+1,0}\} \sim \{u_\varepsilon^n, v_\varepsilon^n\}$ (where $\{u_\varepsilon^n, v_\varepsilon^n\}$ is the approximate solution of (P_ε^{n-1}) or (Q_ε^{n-1})), and we construct the functions $\{u_h^{n+1,k}, v_h^{n+1,k}\}$ as follows :

$$
\int_{\Omega_1} u_h^{n+1,k+1}\cdot\phi_h + \tau\int_{\Omega_1} D_1(u_h^{n+1,k})\nabla u_h^{n+1,k+1}\cdot\nabla\psi_h
$$
$$
+ \int_{\Omega_2} v_h^{n+1,k+1}\cdot\psi_h + \varepsilon\tau D_2\int_{\Omega_2}\nabla v_h^{n+1,k+1}\cdot\nabla\psi_h
$$
$$
= \int_{\Omega_1} u_\varepsilon^n\cdot\phi_h + \int_{\Omega_2} v_\varepsilon^n\cdot\psi_h \qquad \forall\{\phi_h,\psi_h\} \ . \qquad \square
$$

Algorithm (A_{3h}) (Extrapolated Gauss-Seidel-Newton) ; see [9, 10])
Generally speaking, to solve the nonlinear problem in $\mathbb{R}^M$

$$F_i(y_1, y_2, \ldots y_M) = 0 \quad , \quad 1 \le i \le M \ , \tag{5.10}$$

where the functions F_i are sufficiently smooth and the matrix $\left\{\frac{\partial F_i}{\partial y_j}\right\}_{i,j=1}^{M}$ is (say) diagonally dominant, this algorithm gives :

$$\left\{ \begin{array}{l} y_i^{\ell+1} = y_i^{\ell} - \omega \dfrac{F_i(y_1^{\ell+1}, \ldots, y_{i-1}^{\ell+1}, y_i^{\ell}, \ldots, y_M^{\ell})}{\dfrac{\partial F_i}{\partial y_i}(y_1^{\ell+1}, \ldots, y_{i-1}^{\ell+1}, y_i^{\ell}, \ldots, y_M^{\ell})} \\ \\ i = 1, 2, \ldots, M, \quad 0 < \omega < 2 \ . \end{array} \right. \tag{5.11}$$

Notice that problems (5.8) and (5.9) can be written as (5.10) with M being the number of unknown nodal values $u_h(a^k)$ and $v_h(b^\ell)$ and

$$\begin{aligned} F_i &\equiv F_i\Big(\sum_k u_h(a^k)\phi_k^h + \sum_\ell v_h(b^\ell)\psi_\ell^h\Big) \\ &= \int_{\Omega_1} (u_h - u_\varepsilon^n)\phi_i^h + \tau \int_{\Omega_1} D_1(u_h)\nabla u_h \cdot \nabla \phi_i^h \\ &+ \int_{\Omega_2} (v_h - v_\varepsilon^n)\psi^h + \tau D_2 \int_{\Omega_2} \nabla v_h \cdot \nabla \psi_i^h \ . \end{aligned}$$

□

It is readily noticed that for the implementation of these algorithms some quadrature schemes have to be used. For other methods, the reader is referred to [2].

An alternative is provided by the singular perturbation method in Section 4, which can be applied directly on (5.8) or (5.9). This allows to localize the nonlinearity in Ω_1 (in Ω_2 only linear problems have to be solved). For solving (the finite element approximation of) $(4.4)_1$, iterative methods as (A_{1h})-(A_{2h}) can be used, while all the other (linear) problems can be solved by (say) relaxation algorithms.

6. - SOME NUMERICAL EXPERIMENTS AND FURTHER COMMENTS

We turn now to some numerical results concerning problem (Q_ε). We consider the impurity diffusion with segregation phenomena of Arsenic during 120 minutes at 1000° C, in uniformly Boron doped Silicon. It will be assumed for simplicity that the Boron is not active, thus leading to an uncoupled diffusion problem (see [1, 3, 16]). The various constants arising in the definition of the diffusion coefficient D_1 (see Appendix A) have been assigned the following numerical values :

$$z = -1 \quad , \quad z' = +1 \quad ,$$
$$\beta = 100 \ ,$$
$$D_{10}^{o} = 22.9 \exp(-\ 47579.92/T) \ cm^2/s.$$

The intrinsic carrier concentration is given by

$$n_i = 2.09717.10^{16} \ T^{3/2} \exp(-\ 6520/T) \ cm^{-3}$$

and the boron doped substrat is held at

$$10^{15} \ atoms/cm^3.$$

We have fixed the constant C_o (the impurity initial concentration in the oxide "reservoir") equal to 10^{20} (resp. 10^{21}) atoms/cm^3 and the corresponding results are displayed in Fig. 3 to 5 (resp. Fig. 6 and 7). In both cases, the constant m has been (typically) setted equal to .10.

Let us finally make a few comments on the numerical simulation of this kind of problems. First, we recall that these methods also apply to more general situations, such as three-dimensional diffusion of one or several impurities. We also see that the impurity distributions in the Silicon and in the oxide mask are as expected (see [5] for a comparison with one-dimensional related problems), and in particular the transmission conditions on S are well observed.

APPENDIX A : Diffusion coefficients for arsenic and boron in silicon.

The transport of the impurity atoms in Ω_1 is given by the mass continuity equation

$$\frac{\partial u}{\partial t} = - \nabla \cdot \vec{J}_1 \text{ in } \Omega_1 \quad , \tag{A.1}$$

where $\vec{J}_1$ is the density (or impurity flux). Taking into account the electric field enhancement diffusion,

$$\vec{J}_1 = - D_1^o \nabla u + z\mu_1 u\vec{E} \quad , \tag{A.2}$$

where D_1^o is the impurity diffusion coefficient, μ_1 is the mobility, z is the charge and $\vec{E}$ is the electrical field.

Assuming that :

a) Einstein's relation holds good ($D_1 = \frac{kT^*}{q} \mu_1$) ,
b) the global charge density is zero ,
c) the electron and hole populations are in a thermodynamical equilibrium and satisfy Boltzmann's statistics ,

one has :

$$\vec{E} = - \nabla\psi = - \frac{kT}{q} \nabla(\log \frac{n}{n_i}) \quad , \tag{A.3}$$

with ψ, n_i, k and q being resp. the potential, the intrinsic carrier concentration, the Boltzmann's constant and the electron charge. The electron density n is given by

$$n = \frac{1}{2} \{ zu + z'u' + \sqrt{(zu+z'u')^2 + 4n_i^2} \} \quad , \tag{A.4}$$

where u' (resp. z') is the "old" impurity concentration (resp. charge) in Ω_1, and the hole density p satisfies

$$zu + z'u' + p-n = 0 \quad , \quad pn = n_i^2 \quad .$$

To account for charges vancancy reaction (see [11]), we consider the following formulation of D_1^o :

$$(A.5) \qquad D_1^o = D_{10}^o \frac{1+\beta f}{1+\beta} \quad .$$

Here, D_{10}^o is the intrinsic diffusivity corresponding to a very weak concentration, $f = n/n_i$ for donnors (such as arsenic) and $f = p/n_i$ for acceptors (as boron).

Setting

$$(A.6) \qquad D_1(u) = D_{10}^o \frac{1+\beta f}{1+\beta} \left(1 + \frac{u}{\sqrt{(zu+z'u')^2 + 4n_i^2}}\right) ,$$

the continuity equation (A.1) reads :

$$\frac{\partial u}{\partial t} = \nabla\cdot(D_1(u)\ u) \ \underline{\text{in}}\ \Omega_1 .$$

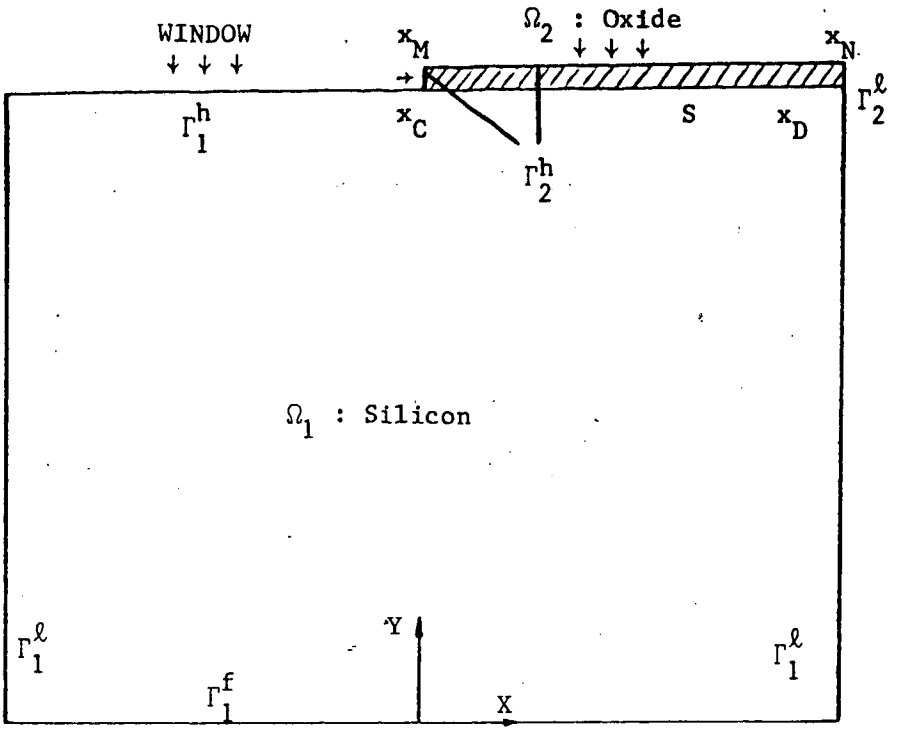


Fig. 1 : The idealized structure

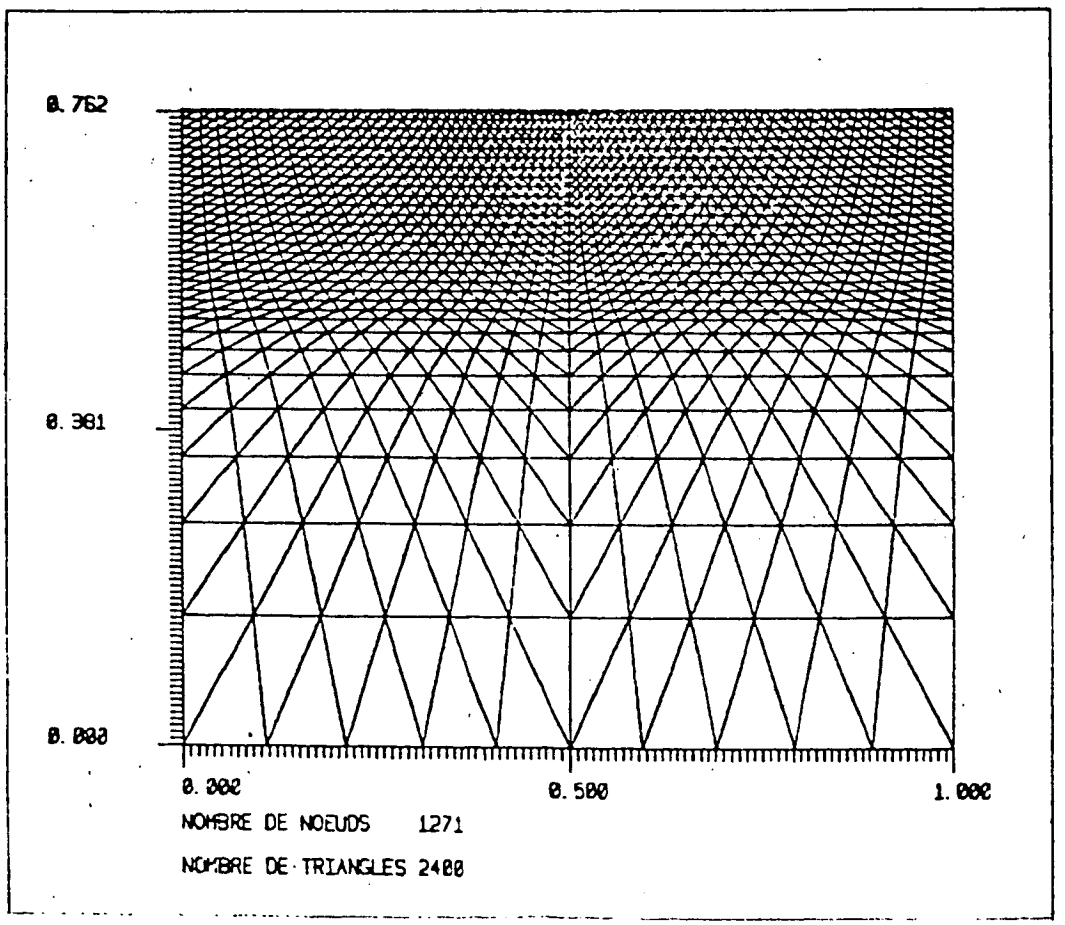
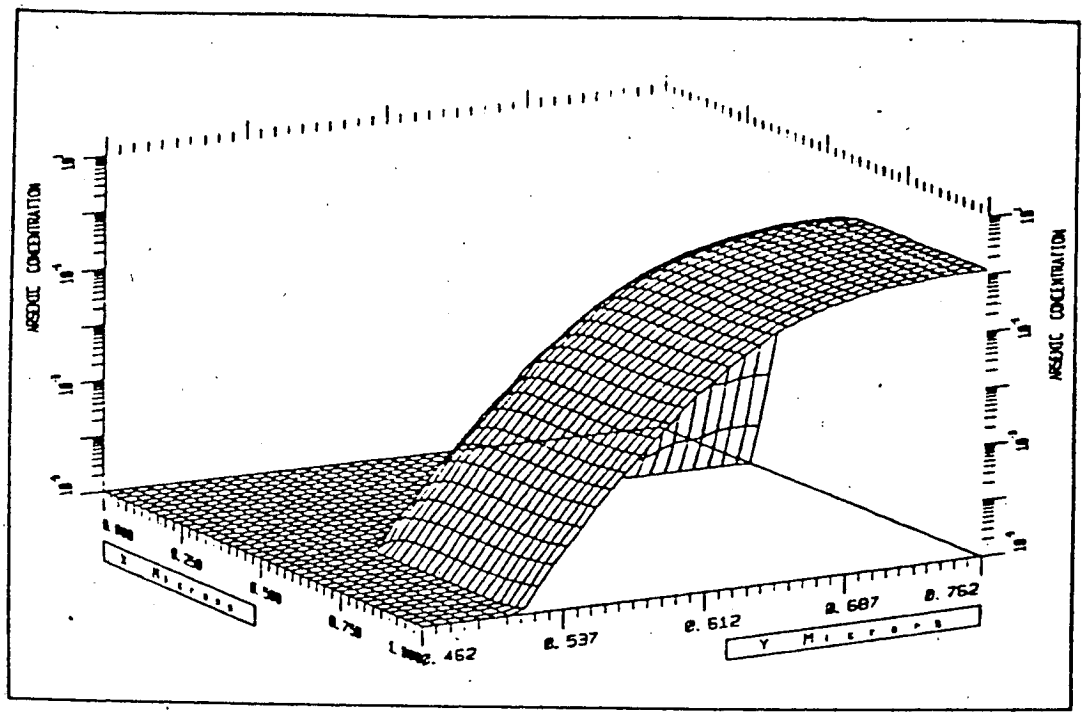
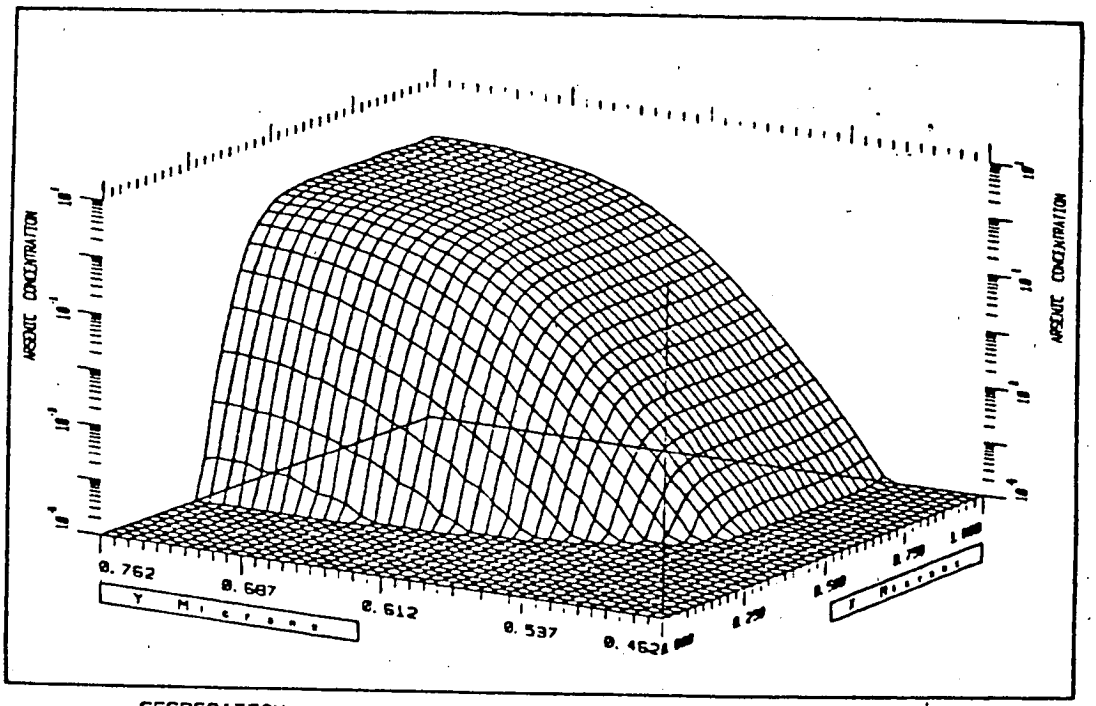


Fig. 2 : The mesh on Ω_1 (Silicon)



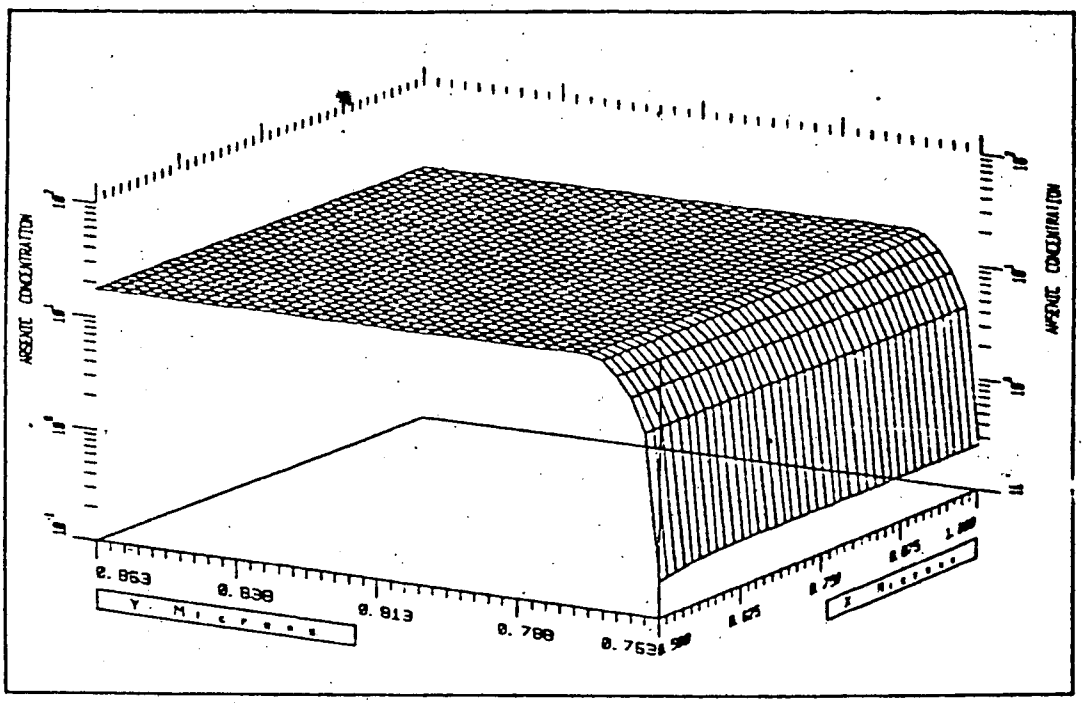
SEGREGATION ARSENIC PLOT (Silicon)
BORON DOPED SUBSTRAT 1E15 cm-3 (1.76E-4)
ARSENIC DOPED OXIDE 1E20 cm-3 (17.6)
PROCESS: 1000 Degrees 2 Hours

Fig. 3 : Impurity concentration in Silicon (1st view).



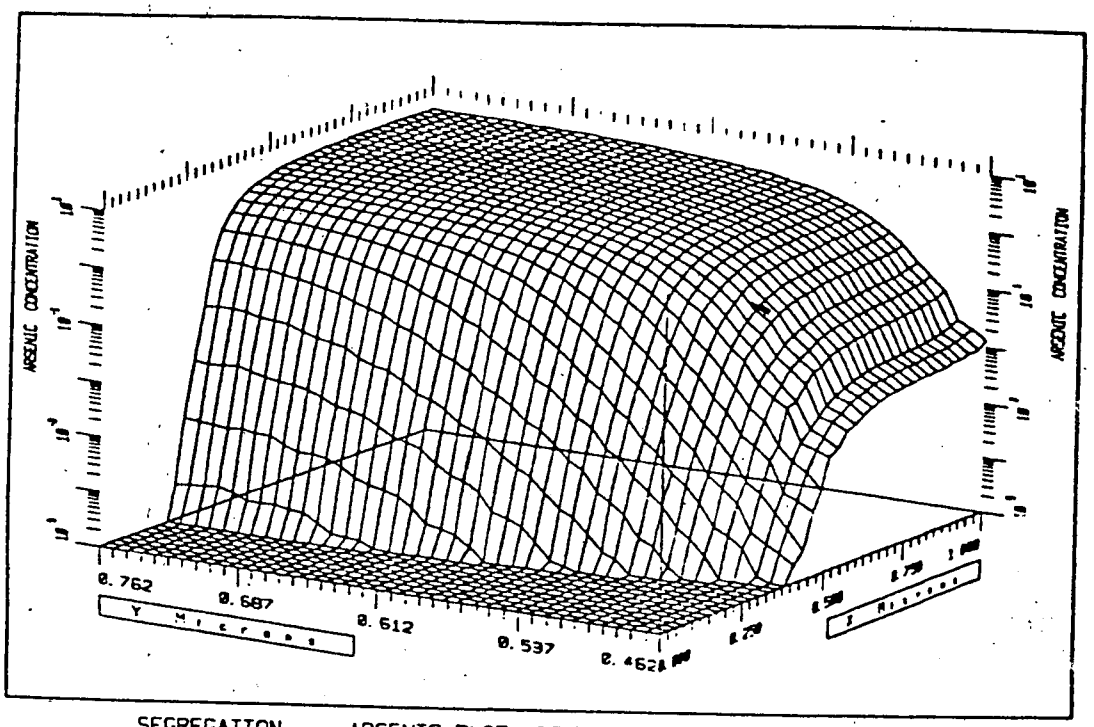
SEGREGATION ARSENIC PLOT (Silicon)
BORON DOPED SUBSTRAT 1E15 cm-3 (1.76E-4)
ARSENIC DOPED OXIDE 1E20 cm-3 (17.6)
PROCESS: 1000 Degrees 2 Hours

Fig. 4 : Impurity concentration in Silicon (2nd view)



SEGREGATION ARSENIC PLOT (Oxide)
BORON DOPED SUBSTRAT 1E15 cm-3 (1.76E-4)
ARSENIC DOPED OXIDE 1E20 cm-3 (17.6)
PROCESS: 1000 Degrees 2 Hours

Fig. 5 : Impurity concentration in the oxide mask.



SEGREGATION ARSENIC PLOT (Silicon)
BORON DOPED SUBSTRAT 1E15 cm-3 (1.76E-4)
ARSENIC DOPED OXIDE 1E21 cm-3 (176.)
PROCESS: 1000 Degrees 2 Hours

Fig. 6 : Impurity concentration in Silicon.

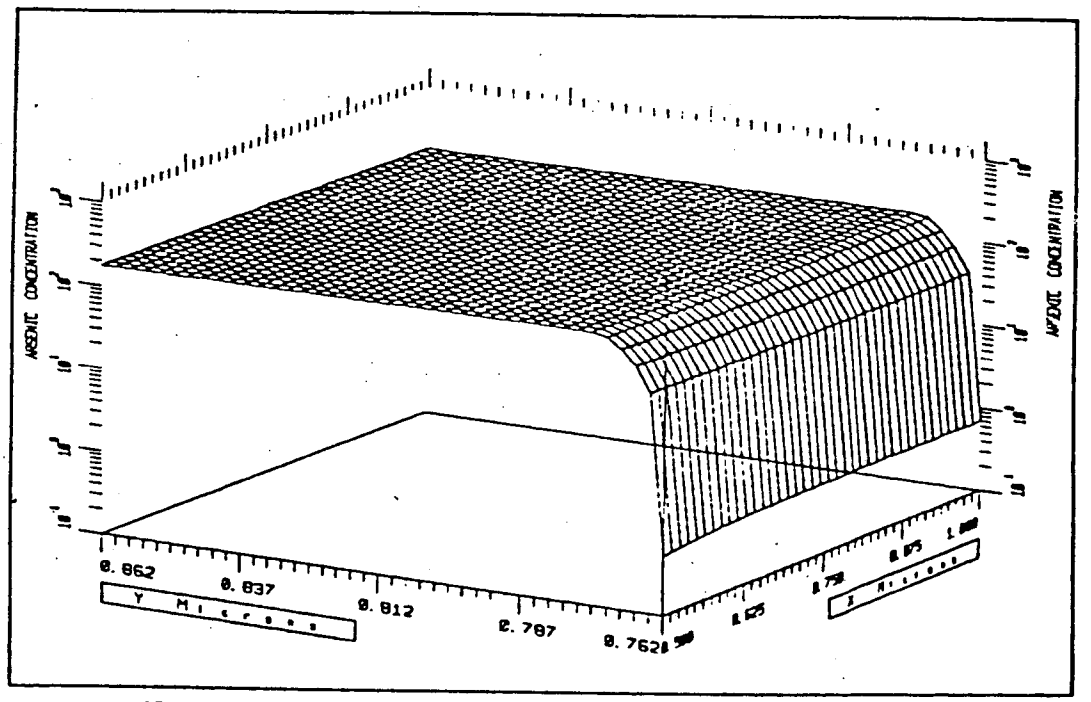


Fig. 7 : Impurity concentration in the oxide mask.

REFERENCES

[1] E. CAQUOT ; E. FERNANDEZ CARA & A. MARROCCO : Résolution numérique d'un problème non linéaire lié à la diffusion d'impuretés dans du Silicium. Proceedings of the "5ème Conférence Internationale sur les Méthodes de Calcul Scientifique et Technique", R. Glowinski & J.L. Lions ed., Versailles, December 1981. North-Holland P. Co., 1982.

[2] E. CAQUOT ; E. FERNANDEZ CARA & A. MARROCCO : 2-D Simulation of coupled diffusion and segregation of impurities in V.L.S.I. process using finite elements. Joint SIAM-IEEE Conference on Numerical Simulation of VLSI Devices, Boston, November 1982.

[3] E. CAQUOT & A. MARROCCO : Numerical simulations with finite elements of nonlinear impurity diffusion in silicon. In "2nd International Conference on the Numerical Analysis of Semiconductor Devices and Integrated Circuits", B.T. Browne & J.J.A. Miller, Boole Press (Dublin), 1981, p. 162-170.

[4] M.G. CRANDALL : Semigroups of nonlinear transformations in Banach spaces. In "Contributions to Nonlinear Functional Analysis". E. Zarantonello ed., New York, Academic Press, 1976, p. 131-165.

[5] R.B. FAIR & J.C.C. TSAI : The diffusion of ionimplanted arsenic in silicon. J. Electrochem. Soc. : Solid-State Sc. Tech., Vol. 122, n° 12 (1975), p. 1689-1696.

[6] E. FERNANDEZ CARA : To appear.

[7] E. FERNANDEZ CARA : A nonlinear diffusion problem arising in semiconductor process modelling with a singularity. Research Report, INRIA, to appear (1982).

[8] P.L. GEORGE : Résolution numérique de problèmes évolutifs. Thèse de 3ème cycle, Paris VI, 1980.

[9] R. GLOWINSKI : La méthode de relaxation. Quaderni dei Rendiconti di Mat. 14, Roma, Instituto Guido Castelnuovo, 1971.

[10] R. GLOWINSKI & A. MARROCCO : Finite element approximation and iterative methods of solution for 2D nonlinear magnetostatic problems. Proceedings of COMPUMAG Conference, Oxford, April 1976, p. 112-125.

[11] S.M. HU : General theory of impurity diffusion in semiconductors via the vacancy mechanism. Phys. Rev. 180 (1969), p. 773-784.

[12] R. KRAFT : Finite- difference techniques for diffusion and redistribution problems with segregation-type boundary conditions. In "Advances in Computer Methods for Partial Differential Equations", R. Vichnevetsky ed., AICA, New Jersey, 1975.

[13] J.L. LIONS : Quelques Méthodes de Résolution des Problèmes aux Limites non Linéaires. Dunod, Gauthier-Villars, Paris 1969.

[14] J.L. LIONS : Perturbations singulières dans les problèmes aux limites et en contrôle optimal. Lecture Notes in Math., n° 323, Springer-Verlag.

[15] G. STAMPACCHIA : Equations elliptiques du second ordre à coefficients discontinus. Séminaire de Mathématiques Supérieures, Université de Montréal, 1966.

[16] D.D. WARNER & C.L. WILSON : Two-dimensional concentration dependent-diffusion. Bell System Tech. J., 59, 1 (1980), p. 1-40.

Imprimé en France

par

l'Institut National de Recherche en Informatique et en Automatique